

Citation for published version:

Li, W, Fukunishi, M, Morgan, B, Borkiewicz, O, Chapman, K, Pralong, V, Maignan, A, Lebedev, O, Ma, J, Groult, H, Komaba, S & Dambournet, D 2017, 'A Reversible Phase Transition for Sodium Insertion in Anatase TiO_2 ', *Chemistry of Materials*, vol. 29, no. 4, pp. 1836-1844. <https://doi.org/10.1021/acs.chemmater.7b00098>

DOI:

[10.1021/acs.chemmater.7b00098](https://doi.org/10.1021/acs.chemmater.7b00098)

Publication date:

2017

Document Version

Early version, also known as pre-print

[Link to publication](https://doi.org/10.1021/acs.chemmater.7b00098)

"This document is the Accepted Manuscript version of a Published Work that appeared in final form in *Chemistry of Materials* copyright © American Chemical Society after peer review and technical editing by the publisher.

To access the final edited and published work see <https://doi.org/10.1021/acs.chemmater.7b00098>

University of Bath

Alternative formats

If you require this document in an alternative format, please contact:
openaccess@bath.ac.uk

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

Take down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Supporting Information

A Reversible Phase Transition for Sodium Insertion in Anatase TiO₂

Wei Li,[†] Mika Fukunishi,[§] Benjamin. J. Morgan,[‡] Olaf J. Borkiewicz,[⊥] Karena W. Chapman,[⊥] Valérie Pralong,[°] Antoine Maignan,[°] Oleg I. Lebedev,[°] Jiwei Ma,[†] Henri Groult,[†] Shinichi Komaba,[§] Damien Dambournet^{†,*}

[†] Sorbonne Universités, UPMC Univ Paris 06, CNRS UMR 8234, Laboratoire PHENIX, 4 place Jussieu, F-75005 Paris, France.

[§] Department of Applied Chemistry, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8601, Japan.

[‡] Department of Chemistry, University of Bath, Claverton Down, BA2 7AY, United Kingdom.

[⊥] X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, United States.

[°] Laboratoire CRISMAT, ENSICAEN, Université de Caen, CNRS, 6 Bd Maréchal Juin, F-14050 Caen, France.

Corresponding Author

* damien.dambournet@upmc.fr

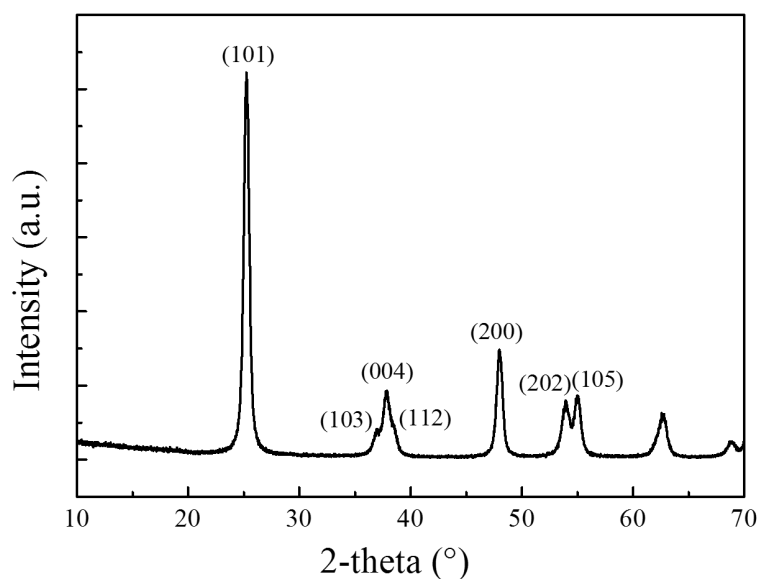


Figure S1. Powder x-ray diffraction pattern of anatase TiO₂.

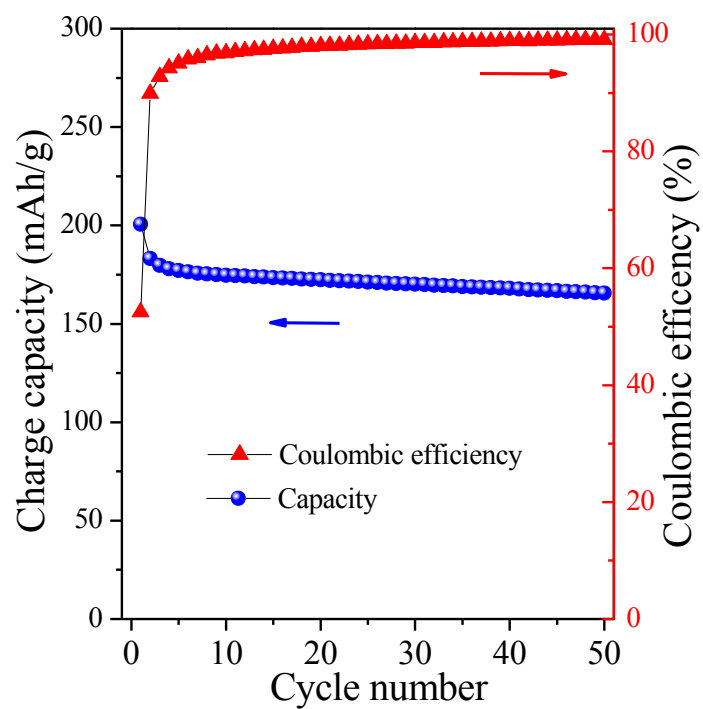


Figure S2. Cycling behavior of anatase TiO_2 upon Na insertion/de-insertion. The capacity obtained after 50 cycles is 165 mAh/g, corresponding to ca. 0.5 Na^+ per TiO_2 .

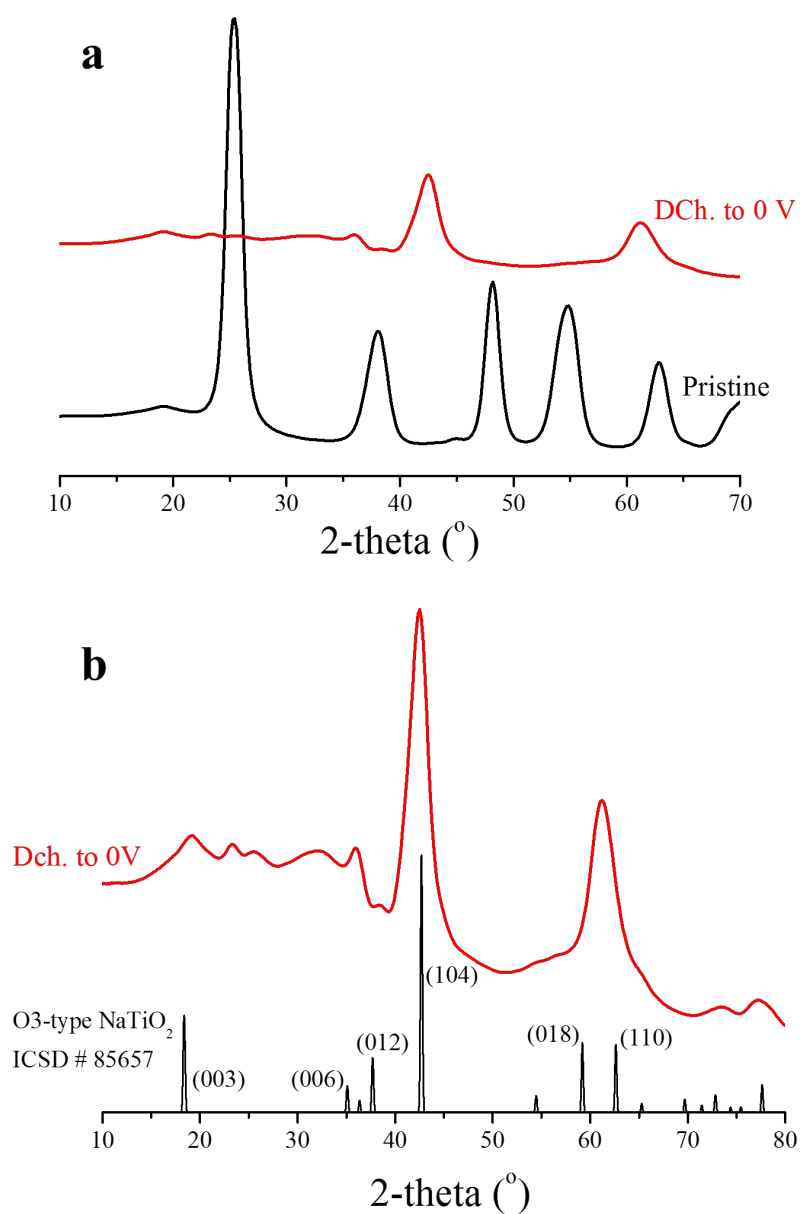


Figure S3. (a) High-energy X-ray diffraction pattern of the pristine and fully discharged TiO_2 electrodes. **(b)** The X-ray diffraction pattern of the fully discharged electrode was indexed with an O3-type NaTiO_2 rhombohedral structure (space group: R-3m).

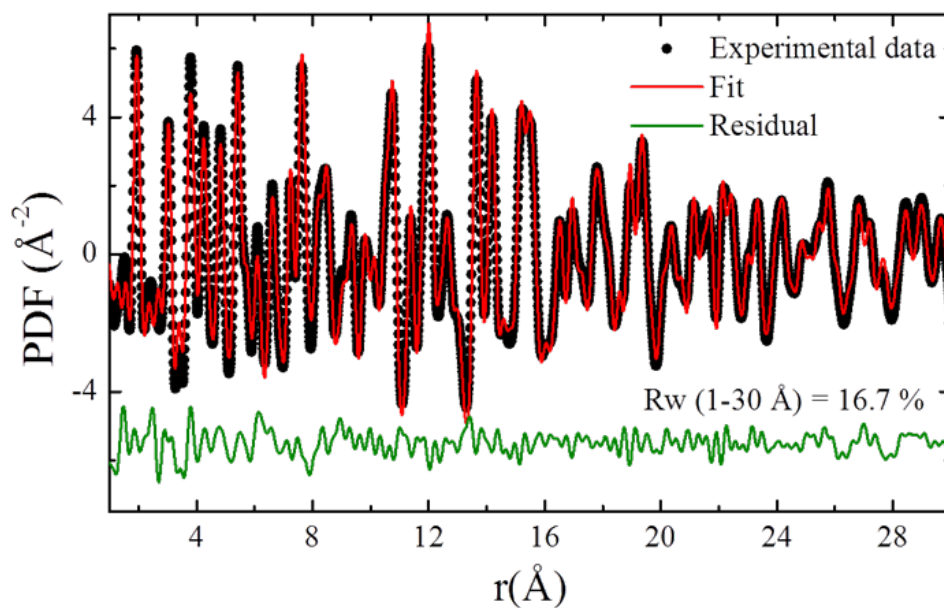


Figure S4. PDF refinement of the TiO_2 electrode discharged to 0.3V, *i.e.* 0.3 Na^+ per TiO_2 .

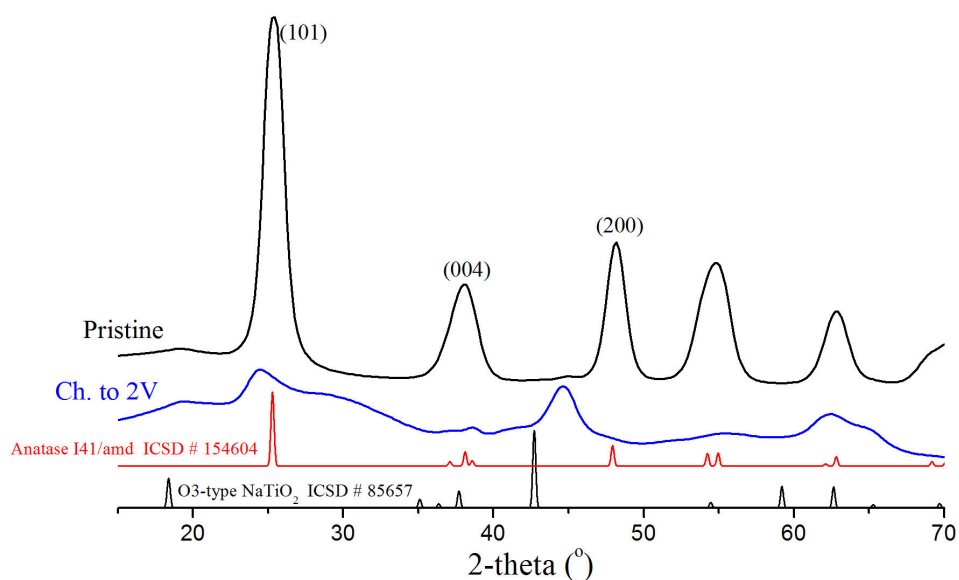


Figure S5. High-energy X-ray diffraction pattern of the fully charged electrode. The peak at $2\text{-theta} \approx 25^\circ$ can be assigned to the (101) of the anatase type structure, indicating the recovery of anatase framework upon charging.

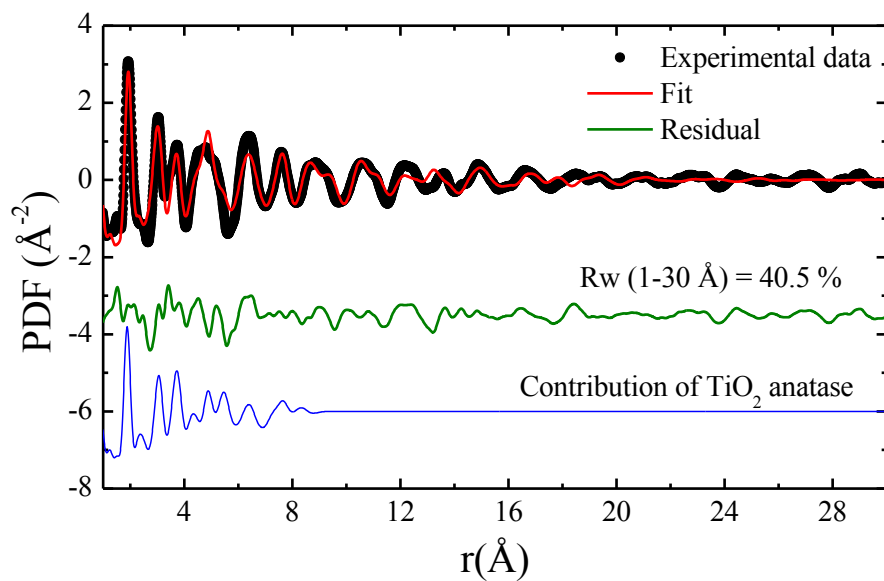


Figure S6. PDF refinement of the electrode charged to 2 V using O3-type NaTiO_2 (space group: R-3m) and TiO_2 (space group: $I4_1/amd$) models. The results show that the desodiated electrode is composed by 20 % O3-type Na_xTiO_2 and 80 % TiO_2 , which agrees with the capacity delivered during the 1st charge. Note that the high value of the Rw is due to strong disorder occurring in Na_xTiO_2 phase.